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SODIUM 2-(2-DODECYLOXYETHOXY)ETHYL SULPHATE
(SODIUM LAURETH SULFATE; CAS NO. 3088-3 1-1):
TEST PLAN

Submitted to the US Environmental Protection Agency

By

Stepan Company

DATE: May 2006

SUMMARY

Stepan Company (**Stepan**) has sponsored Sodium Laureth Sulfate (CAS No. 3088-3 1- 1) under the EPA's High Production Volume (HPV) Program. This document provides the Test Plan and summaries of existing data in support of this substance.

1.0 INTRODUCTION

Stepan has voluntarily committed to participate in the Environmental Protection Agency's (EPA) high production volume chemicals (HPV) challenge program, to assess the health and environmental hazards, including selected physical chemical characteristics of sodium laureth sulfate (CAS No. 3088-3 1-3). Sodium laureth sulfate is an alcohol ethoxysulfate (AES).

An evaluation of the available data and proposed test plan are included in this document. As part of this evaluation, data from structurally analogous substances (other AES) were used to fulfill some endpoints for the sponsored substance (SDA, 1991; HERA, 2003). The HERA has defined the AES family "*to encompass commercial grades of linear-type primary alcohol ethoxysulphates containing AES components of basic structure $C_nH_{2n+1}O(C_2H_4O)_mSO_3X$ where $n=10-18$ and $m = 0-8$ and $X = \text{sodium, ammonium or triethanolamine (TEA)}$* ". Although sodium laureth sulfate was not included in this assessment, it is clearly within the bounds of the HERA definition. In addition to using data from AES, one specific AES (sodium lauryl ether sulfate, SLES, CAS No 9004-82-4) is also used in this assessment. As shown in Figure 1, SLES is a close structural analog of sodium laureth sulfate. Robust summaries for sodium laureth sulfate are provided in Appendix 1. The HERA AES documents are provided in Appendix 2.

The objective of this test plan is to evaluate the available data and determine what additional data, if any, are needed to adequately characterize the physical properties, environmental fate, and human health and environmental effects of sodium laureth sulfate. All endpoints have been fulfilled either with testing completed on the sponsored substance or through the use of testing with structurally analogous AES. No additional testing has been proposed.

Table 1: AVAILABLE DATA FOR SODIUM LAURETH SULFATE

Endpoint	
Physical Chemical Properties	
Melting Point	A (calc)
Vapor Pressure	A (calc)
Boiling Point	A (calc)
Partition Coefficient	A (calc)
Water Solubility	A (calc)
Environmental Fate	
Hydrolysis	A
Photodegradation	A (calc)
Biodegradation	A
Environmental Transport	A (calc)
Ecotoxicity	
Acute/Chronic Fish	R
Acute/Chronic Daphnia	R
Acute/Chronic Algae	R
Mammalian toxicity	
Acute Oral	A
Repeated Dose	R
Genotoxicity (<i>in vitro</i> -bacteria)	R
Genotoxicity (<i>in vivo</i>)	R
Reproductive/Developmental	R

A= Adequate data

Calc = Modeling data

R = Read across to AES

2.0 USE

Sodium laureth sulfate is used in variety of shampoos, bath products, and hand soaps with its good foaming, viscosity building, and low irritation properties (Stepan, 2006a). SLES is used as a scouring, leveling, coupling and foaming agent for textile applications.

3.0 EVALUATION OF EXISTING DATA AND PROPOSED TESTING

Chemical/Physical Prouerties:

Sodium laureth sulfate is a solid. Estimated physical chemical properties are provided in Table 2. The melting point of sodium laureth sulfate is 286 °C (EpiWin v3.11); this is in good agreement with an expected value of greater than 200 (Stepan, 2006b). The boiling point is 659 °C (EpiWin v3.11). A vapor pressure has not been determined but it is expected to be negligible. The estimated vapor pressure is $3.4E^{-15}$ hPa (EpiWin v3.11). The estimated partition coefficient for sodium laureth sulfate is 1.14 (EpiWin v3.11). The estimated water solubility of sodium laureth sulfate is 452 mg/L (EpiWin v3.11), which is in good agreement with the expected value as this substance is very water soluble (Stepan, 2006b).

The physical and chemical properties of analogous AES are summarized in Table 2. The physical chemical properties of sodium laureth sulfate are similar to analogous AES, sodium lauryl ether sulfate (SLES, CAS No 9004-82-4; EpiWin v3.11) and AES(C12) (HERA, 2003).

Table 2: Summary of Physical and Chemical Property Data for Sodium Laureth Sulfate and AES

Compound	Physical Chemical Properties				
	Melting Point (°C)	Boiling Point (°C)	Vapor Pressure (hPa)	Partition Coefficient	Water Solubility
Sodium laureth sulfate	4.4 (freezing point) 287 (estimated)	100 659 (estimated)	3.4E- 15 (estimated)	1.14 (estimated)	452 (estimated)
Supporting data					
AES (as SLES)	290 (estimated)	666 (estimated)	2.01 E-15 (estimated)	1.62 (estimated)	187 (estimated)
AES (C12)	298 (estimated)	684 (estimated)	1.2E-13 (estimated)	0.95 (estimated)	425 (estimated)

Recommendation: No additional testing is proposed.

Environmental Fate.

Environmental fate properties of sodium laureth sulfate and AES/SLES or C 12 are presented in Table 3. Sodium laureth sulfate undergoes 10% decomposition at 1 OOC between 30 and 40 days (Roberts et al.). This is to be expected as an increased rate of hydrolysis is proportional to increases in temperature. Therefore, as temperature decreases, the rate of hydrolysis greatly slows. Under normal use and typical environmental conditions (approximately 25°C at non-catalyzed conditions), this chemical is expected to be resistant to hydrolysis.

Sodium laureth sulfate has been shown to be readily biodegradable (65% after 28 days; AnaylCen, 2003). Photodegradation and fugacity modeling has been conducted for sodium laureth sulfate (EpiWin v3.11). The photodegradation half-life is 0.2 days. Level III fugacity modeling indicates sodium laureth sulfate will partition primarily to soil and water (Air = 0.355%; Water = 49.4%; Soil = 50.1% and Sediment = 0.103%).

AES have been shown to be readily biodegradable, regardless of chain length (HERA, 2003).

Table 3 Summary of Environmental Fate Data for Sodium Laureth Sulfate and AES

Compound	Environmental Fate			
	Stability in Water	Photodegradation	Level III Fugacity Model (%)	Biodegradation
Sodium laureth sulfate	Stable	Rate constant: .00000000045 cm ³ /(molecule*sec) Half-life: .2 days	Air = 0.355 Water = 49.4 Soil = 50.1 Sediment = 0.103	65% after 28 days
SLES	Not applicable	Not applicable	Not applicable	81% after 26 d (S)
AES (C12)	Not applicable	Not applicable	Not applicable	Readily biodegradable

Recommendation: No additional testing is proposed.

Aquatic Toxicity.

Aquatic toxicity data are not available for sodium laureth sulfate. Extensive acute and chronic toxicity data are available for AES (SDA, 1991; HERA, 2003; Warne and Schiffko, 1999). As reported in HERA (2003), there appears to be no difference in sensitivity of fish and invertebrates to AES. Similar effects are expected for the sponsored substance.

Recommendation: No additional testing is proposed.

Table 4 Chronic Aquatic Toxicity Data for Sodium Laureth Sulfate and AES/SLES

Compound	Environmental Effects		
	Fish (mg/L)	Daphnia (mg/L)	Algae (mg/L)
Sodium laureth sulfate	14-day LC50 = 2836 (estimated): read across to AESISLES	No data: read across to AES/SLES	No data: read across to AESISLES
Supporting data			
AES (C12)	<i>Saccobranchus fossilis</i> 60 d > 2.24	<i>C. dubia</i> 7 d NOEC = .34, .88, 1.2, 2.7, 6.3 <i>Brachionus calyciflorus</i> 2 d EC20 = 0.97-1.1, 2.3	<i>S. capricornutum</i> 96 hr NOEC growth = 12 River water 'community' Chlorophyll a NOEC 3 weeks = 70 (enhancement at 5)
AES (C12-14)	<i>Pimephales promelas</i> 96 hr LC50 = 13 (ammonium salt) <i>Lepomis macrochirus</i> 96 hr LC50 = 24 (ammonium salt) <i>Cyprinodon variegatus</i> 96 hr LC50 = 2.3 (ammonium salt)	No data	<i>Selenastrum capricornutum</i> 5 d algistatic = 101, algicidal > 1000
C12-13AE2S	<i>Salmo gairdneri</i> 96 hr LC50 = 28	No data	No data
C12AE2.1S	<i>Lepomis macrochirus</i> 24 hr LC50 = 87	No data	No data
C12AE2S	<i>Pimephales promelas</i> 48 hr LC50 = 1.5	No data	No data
C12-14AE2.2S	No data	<i>Daphnia magna</i> 24 hr EC50 = 21	No data
ammonium C12-14AES	No data	<i>Daphnia magna</i> 96 hr EC50 = 5.7	No data
SLES	No data	<i>Ceriodaphnia dubia</i> 48 hr EC50 = 3.12	No data

Acute Mammalian Toxicity:

Sodium laureth sulfate has a low acute oral toxicity in rats, with an LD50 greater than 5000 mg/kg bw (Hill Top Research, 1982a) (Table 5). The acute oral toxicity of AES is low, with LD50's ranging from 1700 to greater than 5000 mg/kg bw (HERA, 2003). The acute oral toxicity of SLES is also low, with an LD50 of 1600 mg/kg bw (JACT, 1983).

In a semi-occlusive skin irritation study in rabbits, the application of sodium laureth sulfate caused evidence of tissue damage in two of 6 animals (Hill Top Research, 1982b). Atonia, blanching discoloration and spreading of irritative effects was also noted during this study. Application of undiluted sodium laureth sulfate to the right eye of each of 6 rabbits caused evidence of significant corneal, iris and conjunctival changes (Hill Top Research, 1982c).

Recommendation: No additional testing is proposed.

Repeated Dose Toxicity:

Repeated dose toxicity studies have not been conducted with sodium laureth sulfate. Extensive testing has been conducted with AES. One of these studies is summarized here. NaC12-14AE2S was tested for systemic toxicity at repeated doses by oral gavage of 0, 25, 75, and 225 mg/kg bodyweight (HERA, 2003). The compound was administered by gavage for 90 days. Recovery group animals were included in the 0, 75 and 225 mg/kg dose groups. There were no clinical signs, effects on body weight, food or water consumption or body weight gain. The forestomach of the animals of the treated group showed some lesions. A NOEL was not determined, although these effects are not relevant to human health. Based on systemic toxicity, behavioural and clinical abnormalities and other general or specific toxic effects, a no adverse effect level (NOAEL) of 225 mg/kg was established. Additional studies are described in HERA, 2003 (provided as Appendix 2). Overall, these studies indicate no adverse effects, behavioral or clinical abnormalities of AES were observed up to a dose level of 250 mg/kg body weight per day (HERA, 2003). Similar effects are expected for the sponsored substance.

Recommendation: No additional testing is proposed.

Reproductive/Developmental Toxicity:

Reproductive toxicity studies have not been conducted with sodium laureth sulfate. Studies with AES show no reproductive effects. Specifically, a key study has been identified (HERA, 2003). A two generation reproduction study in rats was conducted with NaC12-14AE2S following OECD guideline 4 16. There were no treatment-related reproductive effects at any dose level on the parents or offspring (NOAEL > 3 300 mg/kg/day). The NOAEL for systemic effects of 0.1 % (86.6 mg/kg bw) for the FO generation and a NOAEL of 0.1 % (149.5 mg/kg bw) for the F1 generation was reported (HERA, 2003).

Studies assessing the teratogenic potential and developmental toxicity of AES have been described (HERA, 2003). It was concluded in HERA (2003) "that there is sufficient evidence that AES is not teratogenic or a developmental toxicant under the conditions described. A NOAEL greater than 1000 mg/kg bw/day can be estimated for teratogenicity and embryotoxicity on the basis of the segment II embryotoxicity study which is judged to be of highest reliability. The NOAEL for developmental toxicity appears to be greater than 750 mg/kg bw/day." Similar effects are expected for the sponsored substance.

Recommendation: No additional testing is proposed.

Mutagenicity Assays:

No genetic toxicity testing is available for sodium laureth sulfate. AES have been tested extensively for bacterial and mammalian genotoxicity; results of this testing are consistently negative. It was concluded in HERA (2003) "that there is no evidence that AES are either mutagenic or genotoxic." Similar effects are expected for the sponsored substance.

Recommendation: No additional testing is proposed.

Table 5 Mammalian Toxicity Data for Sodium Laureth Sulfate and AES

Compound	Mammalian Toxicity				
	Oral LD50 (mg/kg)	Repeat Dose Toxicity	Repro. Effects	Develop. Effects	Genetic Toxicity
Sodium laureth sulfate	>5000	No data: read across to AES	No data: read across to AES	No data: read across to AES	No data: read across to AES
Supporting data					
AES	1700 ■ >5000	Rat, 90 day, diet, NOAEL = 225 mg/kg/bw/d *	Rat, two-generation, drinking water, NOAEL (reproduction parent and offspring) > 3% (> 300 mg/kg/bw); NOAEL (FO, systemic) = 0.1 % (86.6 mg/kg bw); NOAEL (F1, systemic) = 0.1 % (149.5 mg/kg bw)	Rat, Segment II, gavage, NOAEL (teratogenicity and embryotoxicity) > 1000 mg/kg bw/day; NOAEL (developmental) > 750 mg/kg bw/day*	Bacterial: negative Mammalian: negative
SLES	1600				

* = AES (NaCl: 4AE2S)

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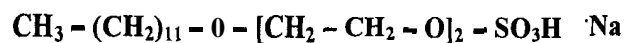
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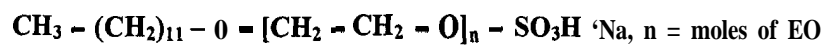


FIGURE I: Structures of Sodium Laureth Sulfate and Sodium Lauryl Ether Sulfate

APPENDIX 1
DOSSIER
SODIUM LAURETH SULFATE

APPENDIX 2
HUMAN & ENVIRONMENTAL RISK ASSESSMENT ON INGREDIENTS OF
EUROPEAN HOUSEHOLD CLEANING PRODUCTS: ALCOHOL
ETHOXYsulphates